Topological Origin of Toughness and Brittleness in Silicate Glasses

Yu, Yingtian; Wang, Bu; Mauro, John C.; Smedskjær, Morten Mattrup; Bauchy, Mathieu

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

Topological Origin of Toughness and Brittleness in Silicate Glasses

Yingtian Yu[1], Bu Wang[1], John C. Mauro[2], Morten M. Smedskjaer[3], Mathieu Bauchy[1]

[1]Civil and Environmental Engineering Department, University of California, Los Angeles, Los Angeles, CA, USA

[2]Corning Incorporated, Corning, NY, USA

[3]Department of Chemistry and Bioscience, Aalborg University, Aalborg, Denmark.

Brittleness is the main limitation of oxide glasses, as impacts, scratching, or vibrations can result in undesirable or even dangerous fracture. As such, increasing the intrinsic ductility of glasses would allow one to design tougher yet transparent materials, which is one of the "Grand Challenges" in glass science. Here, based on molecular dynamics simulations, we show that, despite being brittle at the macroscale, some silicate glasses can feature some ductility at the nanoscale. We demonstrate that a brittle-to-ductile transition can be observed by tuning the topology of the atomic network. Namely, thanks to their internal degrees of freedom, glasses characterized by a flexible network have the ability to undergo local plastic reorganizations, whereas stressed-rigid glasses fail in a brittle way as their network is locked by the high atomic connectivity. Finally, we show that isostatic glasses, which are free of both internal degrees of freedom and eigen-stress, feature an optimal balance between nano-ductility and surface energy and, hence, show maximum fracture toughness. This topological approach could enable the computational design of tough inorganic solids, which has long been a "holy grail" within the non-metallic materials chemistry community.

KEYWORDS: Toughness, Fracture, Ductility, Brittle-to-ductile Transition, Topological constraint theory, Molecular Dynamics.